

Time dependent self-diffusion coefficient of molecules in porous media

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Abstract

Using Monte Carlo simulation, the time dependence of the self-diffusion coefficient $D(t)$ in porous media was investigated. It was found to be a decaying function with a cut-off to zero at time t . The exact form of decay depended on the details of the geometry of porous space. The details of the geometry were described by the surface orientation autocorrelation function. The short-term behavior of $D(t)$ was governed by the surface population of the molecules.

<http://dx.doi.org/10.1063/1.1328416>
